

A direct link between the quantum-mechanical and semiclassical determination of scattering resonances

Andreas Wirzba [‡] and Michael Henseler [§]

Institut für Kernphysik, Technische Universität Darmstadt, Schloßgartenstraße 9,
D-64289 Darmstadt, Germany

Abstract. We investigate the scattering of a point particle from n non-overlapping, disconnected hard disks which are fixed in the two-dimensional plane and study the connection between the spectral properties of the quantum-mechanical scattering matrix and its semiclassical equivalent based on the semiclassical zeta function of Gutzwiller and Voros. We rewrite the determinant of the scattering matrix in such a way that it separates into the product of n determinants of 1-disk scattering matrices – representing the incoherent part of the scattering from the n disk system – and the ratio of two mutually complex conjugate determinants of the genuine multi-scattering kernel, \mathbf{M} , which is of Korringa-Kohn-Rostoker-type and represents the coherent multi-disk aspect of the n -disk scattering. Our result is well-defined at every step of the calculation, as the on-shell \mathbf{T} -matrix and the kernel $\mathbf{M}-\mathbf{1}$ are shown to be trace-class. We stress that the cumulant expansion (which *defines* the determinant over an infinite, but trace class matrix) induces the curvature regularization scheme to the Gutzwiller-Voros zeta function and thus leads to a new, well-defined and direct derivation of the semiclassical spectral function. We show that unitarity is preserved even at the semiclassical level.

PACS numbers: 03.65.Sq, 03.20.+i, 05.45.+b

Short title: A direct link between quantum-mechanical and semiclassical scattering

February 5, 2008

[‡] Andreas.Wirzba@physik.tu-darmstadt.de

[§] Present address: Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany, michael@mpipks-dresden.mpg.de

1. Introduction

In scattering problems whose classical analog is completely hyperbolic or even chaotic, as e.g. n -disk scattering systems, the connection between the spectral properties of exact quantum mechanics and semiclassics has been rather indirect in the past. Mainly the resonance predictions of exact and semiclassical calculations have been compared which of course still is a useful exercise, but does not fully capture the rich structure of the problem. As shown in ref. [1], there exist several semiclassical spectral functions which predict the very same leading resonances but give different results for the phase shifts. Similar results are known for bound systems, see refs. [2, 3]: the comparison of the analytic structure of the pertinent spectral determinant with various semiclassical zeta functions furnishes the possibility of making much more discriminating tests of the semiclassical approximation than the mere comparison of exact eigenvalues with the corresponding semiclassical predictions.

In the exact quantum-mechanical calculations the resonance poles are extracted from the zeros of a characteristic scattering determinant (see e.g. [4]), whereas the semiclassical predictions follow from the zeros (poles) of a semiclassical spectral determinant (trace) of Gutzwiller [5] and Voros [6]. These semiclassical quantities have either been *formally* (i.e. without induced regularization prescription) taken over from bounded problems (where the semiclassical reduction is done via the spectral density) [7, 8] or they have been extrapolated from the corresponding *classical* scattering determinant [9, 10]. Here, our aim is to construct a *direct* link between the quantum-mechanical and the semiclassical treatment of hyperbolic scattering in a concrete context, the n -disk repellers. The latter belong to the simplest realizations of hyperbolic or even chaotic scattering problems, since they have the structure of a quantum billiard — without any confining (outer) walls. Special emphasis is given to a well-defined quantum-mechanical starting-point which allows for the semiclassical reduction *including* the appropriate regularization prescription. In this context the word “direct” refers to a link which is not of *formal* nature, but includes a proper regularization prescription which is *inherited* from quantum mechanics, and not *imposed from the outside by hand*.

The n -disk problem consists in the scattering of a scalar point particle from $n > 1$ circular, non-overlapping, disconnected hard disks which are fixed in the two-dimensional plane. Following the methods of Gaspard and Rice [4] we construct the pertinent on-shell \mathbf{T} -matrix which splits into the product of three matrices $\mathbf{C}(k)\mathbf{M}^{-1}(k)\mathbf{D}(k)$. The matrices $\mathbf{C}(k)$ and $\mathbf{D}(k)$ couple the incoming and outgoing scattering wave (of wave number k), respectively, to *one* of the disks, whereas the matrix $\mathbf{M}(k)$ parametrizes the scattering interior, i.e., the *multi-scattering* evolution in the multi-disk geometry. The understanding is that the resonance poles of the $n > 1$

disk problem can only result from the zeros of the characteristic determinant $\det \mathbf{M}(k)$; see the quantum mechanical construction of Gaspard and Rice [4] for the three-disk scattering system [11, 12, 13, 14]. Their work relates to Berry's application [15, 16] of the Korringa-Kohn-Rostoker (KKR) method [17] to the (infinite) two-dimensional Sinai-billiard problem which in turn is based on Lloyd's multiple scattering method [18, 19] for a finite cluster of non-overlapping muffin-tin potentials in three dimension.

On the semiclassical side, the geometrical primitive periodic orbits (labelled by p) are summed up – including repeats (labelled by r) – in the Gutzwiller-Voros zeta function [5, 6, 9]

$$Z_{GV}(z; k) = \exp \left\{ - \sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{(z^{n_p} t_p(k))^r}{1 - \frac{1}{\Lambda_p^r}} \right\} \quad (1.1)$$

$$= \prod_p \prod_{j=0}^{\infty} \left(1 - \frac{z^{n_p} t_p(k)}{\Lambda_p^j} \right), \quad (1.2)$$

where $t_p(k) = e^{ikL_p - i\nu_p\pi/2} / \sqrt{|\Lambda_p|}$ is the so-called p^{th} cycle, n_p is its topological length and z is a book-keeping variable for keeping track of the topological order. The input is purely geometrical, i.e., the lengths L_p , the Maslov indices ν_p , and the stabilities (the leading eigenvalues of the stability matrices) Λ_p of the p^{th} primitive periodic orbits. Note that both expressions for the Gutzwiller-Voros zeta function, the original one (1.1) and the reformulation in terms of an infinite product (1.2), are purely formal. In general, they may not exist without regularization. (An exception is the non-chaotic 2-disk system, since it has only one periodic orbit, $t_0(k)$.) Therefore, the semiclassical resonance poles are normally computed from $Z_{GV}(z=1; k)$ in the (by hand imposed) curvature expansion [9, 8, 21] up to a given topological length m . This procedure corresponds to a Taylor expansion of $Z_{GV}(z; k)$ in z around $z = 0$ up to order z^m (with z taken to be one at the end):

$$Z_{GV}(z; k) = z^0 - z \sum_{n_p=1} \frac{t_p}{1 - \frac{1}{\Lambda_p}} \quad (1.3)$$

$$- \frac{z^2}{2} \left\{ \sum_{n_p=2} \frac{2t_p}{1 - \frac{1}{\Lambda_p}} + \sum_{n_p=1} \frac{(t_p)^2}{1 - \left(\frac{1}{\Lambda_p}\right)^2} - \sum_{n_p=1} \sum_{n_{p'}=1} \frac{t_p}{1 - \frac{1}{\Lambda_p}} \frac{t_{p'}}{1 - \frac{1}{\Lambda_{p'}}} \right\} + \dots \quad (1.4)$$

This is one way of regularizing the formal expression of the Gutzwiller-Voros zeta function (1.1). The hope is that the limit $m \rightarrow \infty$ exists — at least in the semiclassical regime $\text{Re } k \gg 1/a$ where a is the characteristic length of the scattering potential. We will show below that in the quantum-mechanical analog — the cumulant expansion — this limit can be taken.

As mentioned, the connection between quantum mechanics and semiclassics for these scattering problems has been the comparison of the corresponding resonance poles, the

zeros of the characteristic determinant on the one hand and the zeros of the Gutzwiller-Voros zeta function – in general in the curvature expansion – on the other hand. In the literature (see e.g. [7, 8, 13] based on [22, 23]) this link is motivated by the semiclassical limit of the left hand sides of the Krein-Friedel-Lloyd sum for the [integrated] spectral density [24, 25] and [18, 19]

$$\lim_{\epsilon \rightarrow +0} \lim_{b \rightarrow \infty} \left(N^{(n)}(k + i\epsilon; b) - N^{(0)}(k + i\epsilon; b) \right) = \frac{1}{2\pi} \text{Im Tr} \ln \mathbf{S}(k) , \quad (1.5)$$

$$\lim_{\epsilon \rightarrow +0} \lim_{b \rightarrow \infty} \left(\rho^{(n)}(k + i\epsilon; b) - \rho^{(0)}(k + i\epsilon; b) \right) = \frac{1}{2\pi} \text{Im Tr} \frac{d}{dk} \ln \mathbf{S}(k) . \quad (1.6)$$

See also [26] for a modern discussion of the Krein-Friedel-Lloyd formula and [23, 27] for the connection of the (1.6) to the Wigner time-delay. In this way the scattering problem is replaced by the difference of two bounded circular reference billiards of the same radius b which eventually will be taken to infinity, where one contains in its interior the scattering configuration and the other one is empty. Here, $\rho^{(n)}(k; b)$ [$N^{(n)}(k; b)$] and $\rho^{(0)}(k; b)$ [$N^{(0)}(k; b)$] are the spectral densities [integrated spectral densities] in the presence or absence of the scatterers, respectively. In the semiclassical limit, they will be replaced by a smooth Weyl term and an oscillating periodic orbit sum. Note that the above expressions make only sense for wave numbers k above the real axis. Especially, if k is chosen to be real, ϵ must be greater than zero. Otherwise, the exact left-hand sides would give discontinuous staircase or delta functions, respectively, whereas the right-hand sides are by definition continuous functions of k . Thus, the order of the two limits in (1.5) and (1.6) is important, see, e.g., Balian and Bloch [22] who stress that smoothed level densities should be inserted into the Friedel sums.

We stress that these links are of *indirect* nature, since unregulated expressions for the semiclassical Gutzwiller trace formula for *bound* systems arise on the left-hand sides of the (integrated) Krein-Friedel-Lloyd sums in the semiclassical reduction. Neither the curvature regularization scheme nor other constraints on the periodic orbit sum follow from this in a natural way. Since the indirect link of (1.5) and (1.6) is made with the help of bound systems, the question might arise for instance whether in scattering systems the Gutzwiller-Voros zeta function should be resummed according to Berry and Keating [28] or not. This question is answered by the presence of the $i\epsilon$ term *and* the second limit. The wave number is shifted by this from the real axis into the upper complex k plane. This corresponds to a “de-hermiteization” of the underlying hamiltonian – the Berry-Keating resummation which explicitly makes use of the reality of the eigen-energies of a *bound-system* does not apply here. The necessity of the $+i\epsilon$ in the semiclassical calculation can be understood by purely phenomenological considerations: Without the $+i\epsilon$ term there is no reason why one should be able to neglect spurious periodic orbits which solely exist because of the introduction of the confining boundary. The subtraction of the second (empty) reference system helps just in the removal of those

spurious periodic orbits which never encounter the scattering region. The ones that do so would still survive the first limit $b \rightarrow \infty$, if they were not damped out by the $+\epsilon$ term.

The expression for the integrated spectral densities is further complicated by the fact that the ϵ -limit and the integration do not commute either. As a consequence there appears on the l.h.s. of (1.5) an (in general) undetermined integration constant.

Independently of this comparison via the Krein-Friedel-Lloyd sums, it was shown in [20] that the characteristic determinant $\det \mathbf{M}(k) = \det (\mathbf{1} + \mathbf{A}(k))$ can be re-arranged via $e^{\text{Tr} \ln(\mathbf{1} + \mathbf{A}(k))}$ in a cumulant expansion and that the semiclassical analogs to the first traces, $\text{Tr} (\mathbf{A}^m(k))$ ($m = 1, 2, 3, \dots$), contain (including creeping periodic orbits) the sums of all periodic orbits (with and without repeats) of total topological length m . Thus (1.4) should be directly compared with its quantum analog, the cumulant expansion

$$\det (\mathbf{1} + z\mathbf{A}) = 1 - (-z) \text{Tr} [\mathbf{A}(k)] - \frac{z^2}{2} \left\{ \text{Tr} [\mathbf{A}^2(k)] - [\text{Tr} \mathbf{A}(k)]^2 \right\} + \dots \quad (1.7)$$

The knowledge of the traces is sufficient to organize the cumulant expansion of the determinant

$$\det (\mathbf{1} + z\mathbf{A}) = \sum_{m=0}^{\infty} z^m c_m(\mathbf{A}) \quad (1.8)$$

(with $c_0(\mathbf{A}) \equiv 1$) in terms of a recursion relation for the cumulants (see the discussion of the Plemelj-Smithies formula in the appendix)

$$c_m(\mathbf{A}) = \frac{1}{m} \sum_{k=1}^m (-1)^{k+1} c_{m-k}(\mathbf{A}) \text{Tr} (\mathbf{A}^k) \quad \text{for } m \geq 1. \quad (1.9)$$

In the 2nd paper of [20] the geometrical semiclassical analogs to the first three traces were explicitly constructed for the 2-disk problem. The so-constructed geometrical terms correspond exactly (including all prefactors, Maslov indices, and symmetry reductions) to the once, twice or three-times repeated periodic orbit that is spanned by the two disks. (Note that the two-disk system has only one classical periodic orbit.) In the mean-time, one of us has shown that, with the help of Watson resummation techniques [29, 30] and by complete induction, the semiclassical reduction of the quantum mechanical traces of any non-overlapping $2 \leq n < \infty$ disk system [where in addition grazing or penumbra orbits [31, 32] have to be avoided in order to guarantee unique isolated saddle point contributions] reads as follows [33]

$$(-1)^m \text{Tr} (\mathbf{A}^m(k)) \xrightarrow{\text{s.c.}} \sum_p \sum_{r>0} \delta_{m, rn_p} n_p \frac{t_p(k)^r}{1 - \left(\frac{1}{\Lambda_p}\right)^r} + \text{diffractive creeping orbits}, \quad (1.10)$$

where t_p are periodic orbits of topological length n_p with r repeats. The semiclassical reduction (1.10) holds of course only in the case that $\text{Re } k$ is big enough compared

with the inverse of the smallest length scale. Note that (1.10) does not imply that the semiclassical limit $k \rightarrow \infty$ and the cumulant limit $m \rightarrow \infty$ commute in general, i.e., that the curvature expansion exists. The factor n_p results from the count of the cyclic permutations of a “symbolic word” of length n_p which all label the same primary periodic orbit t_p . As the leading semiclassical approximation to $\text{Tr}(\mathbf{A}^m(k))$ is based on the replacement of the m sums by m integrals which are then evaluated according to the saddle point approximation, the qualitative structure of the r.h.s. of (1.10) is expected. The nontrivial points are the weights, the phases, and the pruning of ghost orbits which according to [33] follows the scheme presented in [15]. In [34, 35, 36] \hbar -corrections to the geometrical periodic orbits were constructed, whereas the authors of [37] extended the Gutzwiller-Voros zeta function to include diffractive creeping periodic orbits as well.

By inserting the semiclassical approximation (1.10) of the traces into the exact recursion relation (1.9), one can find a compact expression of the curvature-regularized version of the Gutzwiller-Voros zeta function [9, 8, 21]:

$$Z_{GV}(z; k) = \sum_{m=0}^{\infty} z^m c_m(\text{s.c.}) , \quad (1.11)$$

(with $c_0(\text{s.c.}) \equiv 1$), where the curvature terms $c_m(\text{s.c.})$ satisfy the semiclassical recursion relation

$$c_m(\text{s.c.}) = -\frac{1}{m} \sum_{k=1}^m c_{m-k}(\text{s.c.}) \sum_p \sum_{r>0} \delta_{k, rn_p} n_p \frac{t_p(k)^r}{1 - \left(\frac{1}{\Lambda_p}\right)^r} \quad \text{for } m \geq 1 . \quad (1.12)$$

Below, we construct explicitly a *direct* link between the full quantum-mechanical \mathbf{S} -matrix and the Gutzwiller-Voros zeta function in the particular case of n -disk scattering. We will show that *all* necessary steps in the quantum-mechanical description are justified. It is demonstrated that the spectral determinant of the n -disk problem splits uniquely into a product of n incoherent one-disk terms and one coherent genuine multi-disk term which under suitable symmetries separates into distinct symmetry classes. Thus, we have found a well-defined starting-point for the semiclassical reduction. Since the \mathbf{T} -matrix and the matrix $\mathbf{A} \equiv \mathbf{M} - \mathbf{1}$ are trace class matrices (i.e., the sum of the diagonal matrix elements is absolutely converging in any orthonormal basis), the corresponding determinants of the n -disk and one-disk \mathbf{S} -matrices and the characteristic matrix \mathbf{M} are guaranteed to exist although they are infinite matrices. The cumulant expansion defines the characteristic determinant and guarantees a finite, unambiguous result. As the semiclassical limit is taken, the defining quantum-mechanical cumulant expansion reduces to the curvature-expansion-regularization of the semiclassical spectral function. It will also be shown that unitarity is preserved at the semiclassical level under the precondition that the curvature sum converges or is suitably truncated. In Appendix A the trace-class properties of all matrices entering the expression for the n -disk \mathbf{S} -matrix will be shown explicitly.

2. Direct link

If one is only interested in spectral properties (i.e., in resonances and not in wave functions) it is sufficient to construct the determinant, $\det \mathbf{S}$, of the scattering matrix \mathbf{S} . The determinant is invariant under any change of a complete basis representing the \mathbf{S} -matrix. (The determinant of \mathbf{S} is therefore also independent of the coordinate system.)

For any non-overlapping system of n -disks (which may even have different sizes, i.e., different disk-radii: a_j , $j = 1, \dots, n$) the \mathbf{S} -matrix can be split up in the following way [38] using the methods and notation of Gaspard and Rice [4] (see also [19]):

$$\mathbf{S}_{mm'}^{(n)}(k) = \delta_{mm'} - i \mathbf{C}_{ml}^j(k) \left\{ \mathbf{M}^{-1}(k) \right\}_{ll'}^{jj'} \mathbf{D}_{l'm'}^{j'}(k), \quad (2.1)$$

where $j, j' = 1, \dots, n$ (with n finite) label the (n) different disks and the quantum numbers $-\infty < m, m', l, l' < +\infty$ refer to a complete set of spherical eigenfunctions, $\{|m\rangle\}$, with respect to the origin of the 2-dimensional plane (repeated indices are of course summed over). The matrices \mathbf{C} and \mathbf{D} can be found in Gaspard and Rice [4]; they depend on the origin and orientation of the global coordinate system of the two-dimensional plane and are separable in the disk index j . They parameterize the coupling of the incoming and outgoing scattering wave, respectively, to the j^{th} disk and describe therefore the single-disk aspects of the scattering of a point particle from the n disks:

$$\mathbf{C}_{ml}^j = \frac{2i}{\pi a_j} \frac{J_{m-l}(kR_j)}{H_l^{(1)}(ka_j)} e^{im\Phi_{R_j}}, \quad (2.2)$$

$$\mathbf{D}_{l'm'}^{j'} = -\pi a_{j'} J_{m'-l'}(kR_{j'}) J_{l'}(ka_{j'}) e^{-im'\Phi_{R_{j'}}}. \quad (2.3)$$

Here R_j and Φ_{R_j} denote the distance and angle, respectively, of the ray from the origin in the 2-dimensional plane to the center of the disk j as measured in the global coordinate system. $H_l^{(1)}(kr)$ is the ordinary Hankel function of first kind and $J_l(kr)$ the corresponding ordinary Bessel function. The matrix \mathbf{M} is the genuine multi-disk “scattering” matrix with eliminated single-disk properties (in the pure 1-disk scattering case \mathbf{M} becomes just the identity matrix) [38]:

$$\mathbf{M}_{ll'}^{jj'} = \delta_{jj'} \delta_{ll'} + (1 - \delta_{jj'}) \frac{a_j}{a_{j'}} \frac{J_l(ka_j)}{H_{l'}^{(1)}(ka_{j'})} H_{l-l'}^{(1)}(kR_{jj'}) \Gamma_{jj'}(l, l'). \quad (2.4)$$

It has the structure of a KKR-matrix (see [15, 16, 19]) and is the generalization of the result of Gaspard and Rice [4] for the equilateral 3-disk system to a general n -disk configuration where the disks can have *different* sizes. Here, $R_{jj'}$ is the separation between the centers of the j th and j' th disk and $R_{jj'} = R_{j'j}$. The matrix $\Gamma_{jj'}(l, l') = e^{i(l\alpha_{j'j} - l'(\alpha_{jj'} - \pi))}$ contains – besides a phase factor – the angle $\alpha_{j'j}$ of the ray from the center of disk j to the center of disk j' as measured in the local (body-fixed) coordinate system of disk j . Note that $\Gamma_{jj'}(l, l') = (-1)^{l-l'} (\Gamma_{j'j}(l', l))^*$. The Gaspard and Rice

prefactors, i.e., $(\pi a/2i)$, of \mathbf{M} are rescaled into \mathbf{C} and \mathbf{D} . The product $\mathbf{CM}^{-1}\mathbf{D}$ corresponds to the three-dimensional result of Lloyd and Smith for the on-shell \mathbf{T} -matrix of a finite cluster of non-overlapping muffin-tin potentials. The expressions of Lloyd and Smith (see (98) of [19] and also Berry's form [15]) at first sight seem to look simpler than ours and the ones of [4] for the 3-disk system, as, e.g., in \mathbf{M} the asymmetric term $a_j J_l(ka_j)/a_{j'} H_l^{(1)}(ka_{j'})$ is replaced by a symmetric combination, $J_l(ka_j)/H_l^{(1)}(ka_j)$. This form, however, is not of trace-class. Thus, manipulations which are allowed within our description are not necessarily allowed in Berry's and Lloyd's formulation. After a *formal* rearrangement of our matrices we can derive the result of Berry and Lloyd. Note, however, that the trace-class property of \mathbf{M} is lost in this formal manipulation, such that the infinite determinant and the corresponding cumulant expansion converge only conditionally, and not absolutely as in our case.

The l -labelled matrices $\mathbf{S}^{(n)} - \mathbf{1}$, \mathbf{C} and \mathbf{D} as well as the $\{l, j\}$ -labelled matrix $\mathbf{M} - \mathbf{1}$ are of "trace-class" (see the appendix for the proofs). A matrix is called "trace-class", if, independently of the choice of the orthonormal basis, the sum of the diagonal matrix elements converges absolutely; it is called "Hilbert-Schmidt", if the sum of the absolute squared diagonal matrix elements converges, see the appendix and M. Reed and B. Simon, Vol.1 and 4 [39, 40] for the definitions and properties of trace-class and Hilbert-Schmidt matrices. Here, we will list only the most important ones: (i) any trace-class matrix can be represented as the product of two Hilbert-Schmidt matrices and any such product is trace-class; (ii) the linear combination of a finite number of trace-class matrices is again trace-class; (iii) the hermitean-conjugate of a trace-class matrix is again trace-class; (iv) the product of two Hilbert-Schmidt matrices or of a trace-class and a bounded matrix is trace-class and commutes under the trace; (v) if \mathbf{B} is trace-class, the determinant $\det(\mathbf{1} + z\mathbf{B})$ exists and is an entire function of z ; (vi) the determinant is invariant under unitary transformations. Therefore for all fixed values of k (except at $k \leq 0$ [the branch cut of the Hankel functions] and the countable isolated zeros of $H_m^{(1)}(ka_j)$ and of $\text{Det}\mathbf{M}(k)$) the following operations are mathematically allowed:

$$\begin{aligned}
\det \mathbf{S}^{(n)} &= \det (\mathbf{1} - i \mathbf{CM}^{-1}\mathbf{D}) = \exp \text{tr} \ln (\mathbf{1} - i \mathbf{CM}^{-1}\mathbf{D}) \\
&= \exp \left\{ - \sum_{N=1}^{\infty} \frac{i^N}{N} \text{tr} \left[(\mathbf{CM}^{-1}\mathbf{D})^N \right] \right\} \\
&= \exp \left\{ - \sum_{N=1}^{\infty} \frac{i^N}{N} \text{Tr} \left[(\mathbf{M}^{-1}\mathbf{DC})^N \right] \right\} \\
&= \exp \text{Tr} \ln (\mathbf{1} - i \mathbf{M}^{-1}\mathbf{DC}) = \text{Det} (\mathbf{1} - i \mathbf{M}^{-1}\mathbf{DC}) \\
&= \text{Det} [\mathbf{M}^{-1}(\mathbf{M} - i \mathbf{DC})]
\end{aligned}$$

$$= \frac{\text{Det}(\mathbf{M} - i\mathbf{DC})}{\text{Det}(\mathbf{M})}. \quad (2.5)$$

Actually, $\det(\mathbf{1} + \mu\mathbf{A}) = \exp\{-\sum_{N=1}^{\infty} \frac{(-\mu)^N}{N} \text{tr}[\mathbf{A}^N]\}$ is only valid for $|\mu \max \lambda_i| < 1$ where λ_i is the i -th eigenvalue of \mathbf{A} . The determinant is directly defined through its cumulant expansion (see equation (188) of [40]) which is therefore the analytical continuation of the $e^{\text{tr log}}$ representation. Thus the $e^{\text{tr log}}$ notation should here be understood as a compact abbreviation for the defining cumulant expansion. The capital index L is a multi-index $L = (l, j)$. On the l.h.s. of (2.5) the determinant and traces are only taken over small l , on the r.h.s. they are taken over multi-indices $L = (l, j)$ (we will use the following convention: $\det \dots$ and $\text{tr} \dots$ refer to the $|m\rangle$ space, $\text{Det} \dots$ and $\text{Tr} \dots$ refer to the multi-spaces). The corresponding complete basis is now $\{|L\rangle\} = \{|m; j\rangle\}$ which now refers to the origin of the j th disk (for fixed j of course) and not to the origin of the 2-dimensional plane any longer. In deriving (2.5) the following facts have been used:

- (a) $\mathbf{D}^j, \mathbf{C}^j$ – if their index j is kept fixed – are of trace class (see the appendix)
- (b) and therefore the product \mathbf{DC} – now in the multi-space $\{|L\rangle\}$ – is of trace-class as long as n is finite (see property (ii)),
- (c) $\mathbf{M} - \mathbf{1}$ is of trace-class (see the appendix). Thus the determinant $\text{Det } \mathbf{M}(k)$ exists.
- (d) \mathbf{M} is bounded, since it is the sum of a bounded and a trace-class matrix.
- (e) \mathbf{M} is invertible everywhere where $\text{Det} \mathbf{M}(k)$ is defined (which excludes a countable number of zeros of the Hankel functions $H_m^{(1)}(ka_j)$ and the negative real k axis, since there is a branch cut) and nonzero (which excludes a countable number of isolated points in the lower k -plane) – see the appendix for these properties. Therefore and because of (d) the matrix \mathbf{M}^{-1} is bounded.
- (f) $\mathbf{CM}^{-1}\mathbf{D}$, $\mathbf{M}^{-1}\mathbf{DC}$ are all of trace-class, since they are the product of bounded times trace-class matrices, and $\text{tr}[(\mathbf{CM}^{-1}\mathbf{D})^N] = \text{Tr}[(\mathbf{M}^{-1}\mathbf{DC})^N]$, because such products have the cyclic permutation property under the trace (see properties (ii) and (iv)).
- (g) $\mathbf{M} - i\mathbf{DC} - \mathbf{1}$ is of trace-class because of the rule that the sum of two trace-class matrices is again trace-class (see property (ii)).

Thus all the traces and determinants appearing in (2.5) are well-defined, except at the above mentioned k values. Note that in the $\{|m; j\rangle\}$ basis the trace of $\mathbf{M} - \mathbf{1}$ vanishes trivially because of the $\delta_{jj'}$ terms in (2.4). This does not prove the trace-class property of $\mathbf{M} - \mathbf{1}$, since the finiteness (here vanishing) of $\text{Tr}(\mathbf{M} - \mathbf{1})$ has to be shown for every complete orthonormal basis. After symmetry reduction (see below) $\text{Tr}(\mathbf{M} - \mathbf{1})$, calculated for any irreducible representation, does not vanish any longer. However,

the sum of the traces of all irreducible representations weighted by their pertinent degeneracies still vanishes of course. Semiclassically, this corresponds to the fact that only in the fundamental domain there can exist one-letter “symbolic words”.

Now, the computation of the determinant of the \mathbf{S} -matrix is very much simplified in comparison with the original formulation, since the last term of (2.5) is completely written in terms of closed form expressions and does not involve \mathbf{M}^{-1} any longer. Furthermore, using the notation of Gaspard and Rice [4], one can easily construct

$$\begin{aligned} \mathbf{M}_{ll'}^{jj'} - i \mathbf{D}_{lm'}^j \mathbf{C}_{m'l'}^{j'} &= \delta_{jj'} \delta_{ll'} \left(-\frac{H_{l'}^{(2)}(ka_{j'})}{H_{l'}^{(1)}(ka_{j'})} \right) \\ &\quad - (1 - \delta_{jj'}) \frac{a_j}{a_{j'}} \frac{J_l(ka_j)}{H_{l'}^{(1)}(ka_{j'})} H_{l-l'}^{(2)}(kR_{jj'}) \Gamma_{jj'}(l, l'), \end{aligned} \quad (2.6)$$

where $H_m^{(2)}(kr)$ is the Hankel function of second kind. Note that $\{H_m^{(2)}(z)\}^* = H_m^{(1)}(z^*)$. The scattering from a single disk is a separable problem and the \mathbf{S} -matrix for the 1-disk problem with the center at the origin reads

$$\mathbf{S}_{ll'}^{(1)}(ka) = -\frac{H_l^{(2)}(ka)}{H_l^{(1)}(ka)} \delta_{ll'}. \quad (2.7)$$

This can be seen by comparison of the general asymptotic expression for the wavefunction with the exact solution for the 1-disk problem [38]. Using (2.6) and (2.7) and trace-class properties of $\mathbf{M} - \mathbf{1}$, $\mathbf{M} - i\mathbf{DC} - \mathbf{1}$ and $\mathbf{S}^{(1)} - \mathbf{1}$ one can easily rewrite the r.h.s. of (2.5) as

$$\det \mathbf{S}^{(n)}(k) = \frac{\text{Det}(\mathbf{M}(k) - i\mathbf{D}(k)\mathbf{C}(k))}{\text{Det}\mathbf{M}(k)} = \left\{ \prod_{j=1}^n \left(\det \mathbf{S}^{(1)}(ka_j) \right) \right\} \frac{\text{Det}\mathbf{M}(k^*)^\dagger}{\text{Det}\mathbf{M}(k)}, \quad (2.8)$$

where now the zeros of the Hankel functions $H_m^{(2)}(ka_j)$ have to be excluded as well. In general, the single disks have different sizes. Therefore they are labelled by the index j . Note that the analogous formula for the three-dimensional scattering of a point particle from n non-overlapping balls (of different sizes in general) is structurally completely the same [38, 41] (except that the negative k -axis is not excluded since the spherical Hankel functions have no branch cut). In the above calculation it was used that $\Gamma_{jj'}^*(l, l') = \Gamma_{jj'}(-l, -l')$ in general [38] and that for symmetric systems (equilateral 3-disk-system with identical disks, 2-disk with identical disks): $\Gamma_{jj'}^*(l, l') = \Gamma_{j'j}(l, l')$ (see [4]). The right-hand side of eq.(2.8) is the starting point for the semiclassical reduction, as every single term is guaranteed to exist. The properties of (2.8) can be summarized as follows:

1. The product of the n 1-disk determinants in (2.8) results from the incoherent scattering where the n -disk problem is treated as n single-disk problems.
2. The whole expression (2.8) respects unitarity, since $\mathbf{S}^{(1)}$ is unitary by itself [because of

$\{H_m^{(2)}(z)\}^* = H_m^{(1)}(z^*)$ and since the quotient on the r.h.s. of (2.8) is manifestly unitary. 3. The determinants on the r.h.s. in (2.8) run over the multi-index L . This is the proper form to make the symmetry reductions in the multi-space, e.g., for the equilateral 3-disk system (with disks of the same size) we have

$$\text{Det}\mathbf{M}_{3\text{-disk}} = \det \mathbf{M}_{A1} \det \mathbf{M}_{A2} (\det \mathbf{M}_E)^2, \quad (2.9)$$

and for the 2-disk system (with disks of the same size)

$$\text{Det}\mathbf{M}_{2\text{-disk}} = \det \mathbf{M}_{A1} \det \mathbf{M}_{A2} \det \mathbf{M}_{B1} \det \mathbf{M}_{B2}, \quad (2.10)$$

etc. In general, if the disk configuration is characterized by a finite point symmetry group \mathcal{G} , we have

$$\text{Det}\mathbf{M}_{n\text{-disk}} = \prod_r (\det \mathbf{M}_{D_r}(k))^{d_r}, \quad (2.11)$$

where the index r runs over all conjugate classes of the symmetry group \mathcal{G} and D_r is the r^{th} representation of dimension d_r [38]. [See [42] for notations and [43, 44] for the semiclassical analog.] A simple check that $\text{Det}\mathbf{M}(k)$ has been split up correctly is the power of $H_m^{(1)}(ka_j)$ Hankel functions (for fixed m with $-\infty < m < +\infty$) appearing in the denominator of $\prod_r (\det \mathbf{M}_{D_r}(k))^{d_r}$ which has to be the same as in $\text{Det}\mathbf{M}(k)$ which in turn has to be the same as in $\prod_{j=1}^n (\det \mathbf{S}^{(1)}(ka_j))$. Note that on the l.h.s. the determinants are calculated in the multi-space $\{L\}$. If the n -disk system is totally symmetric, i.e, none of the disks are special in size and position, the reduced determinants on the r.h.s. are calculated in the normal (desymmetrized) space $\{l\}$, however, now with respect to the origin of the disk in the fundamental domain and with ranges given by the corresponding irreducible representations. If some of the n -disk are still special in size or position (e.g., three equal disks in a row [45]), the determinants on the r.h.s. refer to a corresponding symmetry-reduced multi-space. This is the symmetry reduction on the exact quantum-mechanical level. The symmetry reduction can be most easily shown if one uses again the trace-class properties of $\mathbf{M} - \mathbf{1} \equiv \mathbf{A}$

$$\begin{aligned} \text{Det}\mathbf{M} &= \exp \left\{ - \sum_{N=1}^{\infty} \frac{(-1)^N}{N} \text{Tr} [\mathbf{A}^N] \right\} = \exp \left\{ - \sum_{N=1}^{\infty} \frac{(-1)^N}{N} \text{Tr} [\mathbf{U} \mathbf{A}^N \mathbf{U}^\dagger] \right\} \\ &= \exp \left\{ - \sum_{N=1}^{\infty} \frac{(-1)^N}{N} \text{Tr} [(\mathbf{U} \mathbf{A} \mathbf{U}^\dagger)^N] \right\} = \exp \left\{ - \sum_{N=1}^{\infty} \frac{(-1)^N}{N} \text{Tr} [\mathbf{A}_{\text{block}}^N] \right\}, \end{aligned}$$

where \mathbf{U} is unitary transformation which makes \mathbf{A} block-diagonal in a suitable basis spanned by the complete set $\{|m; j\rangle\}$. These operations are allowed because of the trace-class-property of \mathbf{A} and the boundedness of the unitary matrix \mathbf{U} (see the appendix).

As the right-hand side of eq.(2.8) splits into a product of one-disk determinants and the ratio of two mutually complex conjugate genuine n -disk determinants, which are all well defined individually, the semiclassical reduction can be performed for the one-disk

and the genuine multi-disk determinants separately. In [33] the semiclassical expression for the determinant of the 1-disk \mathbf{S} -matrix is constructed in analogous fashion to the semiclassical constructions of [20]:

$$\det \mathbf{S}^{(1)}(ka) \approx \left\{ e^{-i\pi N(ka)} \right\}^2 \frac{\left\{ \prod_{\ell=1}^{\infty} [1 - e^{-i2\pi \bar{\nu}_{\ell}(ka)}] \right\}^2}{\left\{ \prod_{\ell=1}^{\infty} [1 - e^{+i2\pi \nu_{\ell}(ka)}] \right\}^2} \quad (2.12)$$

with the creeping term [30, 37]

$$\nu_{\ell}(ka) = ka + e^{+i\pi/3}(ka/6)^{1/3}q_{\ell} + \dots = ka + i\alpha_{\ell}(ka) + \dots, \quad (2.13)$$

$$\bar{\nu}_{\ell}(ka) = ka + e^{-i\pi/3}(ka/6)^{1/3}q_{\ell} + \dots = ka - i(\alpha_{\ell}(k^*a))^* + \dots = [\nu_{\ell}(k^*a)]^*, \quad (2.14)$$

and $N(ka) = (\pi a^2 k^2)/4\pi + \dots$ being the leading term in the Weyl approximation for the staircase function of the wave number eigenvalues in the disk interior. From the point of view of the scattering particle the interior domains of the disks are excluded relatively to the free evolution without scattering obstacles (see, e.g., [7]), hence the negative sign in front of the Weyl term. For the same reason the subleading boundary term has a Neumann structure, although the disks themselves obey Dirichlet boundary conditions. Let us abbreviate the r.h.s. of (2.12) for a specified disk j as

$$\det \mathbf{S}^{(1)}(ka_j) \xrightarrow{\text{s.c.}} \left\{ e^{-i\pi N(ka_j)} \right\}^2 \frac{\tilde{Z}_l^{(1)}(k^*a_j)^*}{\tilde{Z}_l^{(1)}(ka_j)} \frac{\tilde{Z}_r^{(1)}(k^*a_j)^*}{\tilde{Z}_r^{(1)}(ka_j)}, \quad (2.15)$$

where $\tilde{Z}_l^{(1)}(ka_j)$ and $\tilde{Z}_r^{(1)}(ka_j)$ are the *diffractional* zeta functions (here and in the following semiclassical zeta functions *with* diffractive corrections shall be labelled by a tilde) for creeping orbits around the j th disk in the *left*-handed sense and the *right*-handed sense, respectively.

The genuine multi-disk determinant $\text{Det} \mathbf{M}(k)$ (or $\det \mathbf{M}_{D_r}(k)$ in the case of symmetric disk configurations) is organized according to the cumulant expansion (1.8) which, in fact, *is* the defining prescription for the evaluation of the determinant of an infinite matrix under trace-class property. Thus, the cumulant arrangement is automatically imposed onto the semiclassical reduction. Furthermore, the quantum-mechanical cumulants satisfy the Plemelj-Smithies recursion relation (1.9) and can therefore solely be expressed by the quantum-mechanical traces $\text{Tr} \mathbf{A}^m(k)$. In ref. [33] the semiclassical reduction of the traces, see eq.(1.10), has been derived. If this result is inserted back into the Plemelj-Smithies recursion formula, the semiclassical equivalent of the exact cumulants arise. These are nothing but the semiclassical curvatures (1.12), see [9, 8, 21]. Finally, after the curvatures are summed up according to eq.(1.11), it is clear that the semiclassical reductions of the determinants in (2.8) or (2.11) are the Gutzwiller-Voros spectral determinants (with creeping corrections) in the curvature-expansion-regularization. In the case where intervening disks “block out” ghost orbits [15, 46]), the corresponding orbits have to be pruned, see [33]. In summary,

we have

$$\text{Det}\mathbf{M}(k) \xrightarrow{\text{s.c.}} \tilde{Z}_{GV}(k)|_{\text{curv. reg.}}, \quad (2.16)$$

$$\det \mathbf{M}_{D_r}(k) \xrightarrow{\text{s.c.}} \tilde{Z}_{D_r}(k)|_{\text{curv. reg.}} \quad (2.17)$$

where creeping corrections are included in the semiclassical zeta functions. The semiclassical limit of the r.h.s. of (2.8) is

$$\begin{aligned} \det \mathbf{S}^{(n)}(k) &= \left\{ \prod_{j=1}^n \det \mathbf{S}^{(1)}(ka_j) \right\} \frac{\text{Det}\mathbf{M}(k^*)^\dagger}{\text{Det}\mathbf{M}(k)} \\ &\xrightarrow{\text{s.c.}} \left\{ \prod_{j=1}^n \left(e^{-i\pi N(ka_j)} \right)^2 \frac{\tilde{Z}_l^{(1)}(k^*a_j)^*}{\tilde{Z}_l^{(1)}(ka_j)} \frac{\tilde{Z}_r^{(1)}(k^*a_j)^*}{\tilde{Z}_r^{(1)}(ka_j)} \right\} \frac{\tilde{Z}_{GV}(k^*)^*}{\tilde{Z}_{GV}(k)}, \end{aligned} \quad (2.18)$$

where we now suppress the qualifier $\cdots|_{\text{curv. reg.}}$. For systems which allow for complete symmetry reductions (i.e., equivalent disks with $a_j = a \ \forall j$.) the semiclassical reduction reads

$$\begin{aligned} \det \mathbf{S}^{(n)}(k) &= \left\{ \det \mathbf{S}^{(1)}(ka) \right\}^n \frac{\prod_r \left\{ \det \mathbf{M}_{D_r}(k^*)^\dagger \right\}^{d_r}}{\prod_r \left\{ \det \mathbf{M}_{D_r}(k) \right\}^{d_r}} \\ &\xrightarrow{\text{s.c.}} \left\{ e^{-i\pi N(ka)} \right\}^{2n} \left\{ \frac{\tilde{Z}_l^{(1)}(k^*a)^*}{\tilde{Z}_l^{(1)}(ka)} \frac{\tilde{Z}_r^{(1)}(k^*a)^*}{\tilde{Z}_r^{(1)}(ka)} \right\}^n \frac{\prod_r \left\{ \tilde{Z}_{D_r}(k^*)^* \right\}^{d_r}}{\prod_r \left\{ \tilde{Z}_{D_r}(k) \right\}^{d_r}} \end{aligned} \quad (2.19)$$

in obvious correspondence. [See [43, 44] for the symmetry reductions of the Gutzwiller-Voros zeta function.] These equations do not only give a relation between exact quantum mechanics and semiclassics at the poles, but for *any* value of k in the allowed k region (e.g., $\text{Re } k > 0$). There is the caveat that the semiclassical limit and the cumulant limit might not commute in general and that the curvature expansion has a finite domain of convergence [9, 10, 47].

It should be noted that for *bound* systems the idea to focus not only on the positions of the zeros (eigenvalues) of the zeta functions, but also on their analytic structure and their values taken elsewhere was studied in refs. [2, 3].

3. Discussion

We have shown that (2.8) is a well-defined starting-point for the investigation of the spectral properties of the exact quantum-mechanical scattering of a point particle from a finite system of non-overlapping disks in 2 dimensions. The genuine coherent multi-disk scattering decouples from the incoherent superposition of n single-disk problems. We furthermore demonstrated that (2.18) [or, for symmetry-reducible problems, equation (2.19)] closes the gap between the quantum mechanical and the semiclassical description of these problems. Because the link involves determinants of infinite matrices with

trace-class kernels, the defining cumulant expansion automatically induces the curvature expansion for the semiclassical spectral function. We have also shown that in n -disk scattering systems unitarity is preserved on the semiclassical level.

The result of (2.18) is compatible with Berry's expression for the integrated spectral density in Sinai's billiard (a *bound* $n \rightarrow \infty$ disk system, see equation (6.11) of [15]) and – in general – with the Krein-Friedel-Lloyd sums (1.5). However, all the factors in the first line of the expressions (2.18) and (2.19) are not just of formal nature, but shown to be *finite* except at the zeros of the Hankel functions, $H_m^{(1)}(ka)$ and $H_m^{(2)}(ka)$, at the zeros of the various determinants and on the negative real k axis, since $\mathbf{M}(k) - \mathbf{1}$ and $\mathbf{S}^{(1)}(k) - \mathbf{1}$ are “trace-class” almost everywhere in the complex k -plane.

The semiclassical expressions (second lines of (2.18) and (2.19)) are finite, if the zeta functions follow the induced curvature expansion and if the limit $m \rightarrow \infty$ exists also semiclassically [the curvature limit $m \rightarrow \infty$ and the semiclassical limit $\text{Re } k \rightarrow \infty$ do not have to commute]. The curvature regularization is the semiclassical analog to the well-defined quantum-mechanical cumulant expansion. This justifies the formal manipulations of [7, 8, 48].

Furthermore, even semiclassically, unitarity is automatically preserved in scattering problems (without any reliance on re-summation techniques à la Berry and Keating[28] which are necessary and only applicable in bound systems), since

$$\det \mathbf{S}^{(n)}(k)^\dagger = \frac{1}{\det \mathbf{S}^{(n)}(k^*)} \quad (3.1)$$

is valid both quantum-mechanically (see the first lines of (2.18) and (2.19)) and semiclassically (see the second lines of (2.18) and (2.19)). There is the caveat that the curvature-regulated semiclassical zeta function has a finite domain of convergence defined by the poles of the dynamical zeta function in the lower complex k -plane [9, 10, 47]. Below this boundary line the semiclassical zeta function has to be truncated at finite order in the curvature expansion [1]. Thus, under the stated conditions unitarity is preserved for n -disk scattering systems on the semiclassical level. On the other hand, unitarity can therefore not be used in scattering problems to gain any constraints on the structure of \tilde{Z}_{GV} as it could in bound systems, see [28].

To each (quantum-mechanical or semiclassical) pole of $\det \mathbf{S}^{(n)}(k)$ in the lower complex k -plane determined by a zero of $\text{Det} \mathbf{M}(k)$ there belongs a zero of $\det \mathbf{S}(k)$ in the upper complex k -plane (determined by a zero of $\text{Det} \mathbf{M}(k^*)$ with the same $\text{Re } k$ value, but opposite $\text{Im } k$). We have also demonstrated that the zeta functions of the pure 1-disk scattering and the genuine multi-disk scattering decouple, i.e., the 1-disk poles do not influence the position of the *genuine* multi-disk poles. However, $\text{Det} \mathbf{M}(k)$ does not only possess zeros, but also poles. The latter exactly cancel the poles of the product of the 1-disk determinants, $\prod_{j=1}^n \det \mathbf{S}^{(1)}(ka_j)$, since both involve the same “number” and “power” of $H_m^{(1)}(ka_j)$ Hankel functions in the denominator. The same

is true for the poles of $\text{Det}\mathbf{M}(k^*)^\dagger$ and the *zeros* of $\prod_{j=1}^n \det \mathbf{S}^{(1)}(ka_j)$, since in this case the “number” of $H_m^{(2)}(ka_j)$ Hankel functions in the denominator of the former and the numerator of the latter is the same — see also Berry’s discussion on the same cancellation in the integrated spectral density of Sinai’s billiard, equation (6.10) of [15]. Semiclassically, this cancellation corresponds to a removal of the additional creeping contributions of topological length zero, $1/(1 - \exp(i2\pi\nu_\ell))$, from \tilde{Z}_{GV} by the 1-disk diffractive zeta functions, $\tilde{Z}_l^{(1)}$ and $\tilde{Z}_r^{(1)}$. The orbits of topological length zero result from the geometrical sums over additional creepings around the single disks, $\sum_{n_w=0}^\infty (\exp(i2\pi\nu_\ell))^{n_w}$ (see [37]). They multiply the ordinary creeping paths of non-zero topological length. Their cancellation is very important in situations where the disks nearly touch, since in such geometries the full circulations of creeping orbits around any of the touching disks should clearly be suppressed, as it now is. Therefore, it is important to keep consistent account of the diffractive contributions in the semiclassical reduction. Because of the decoupling of the one-disk from the multi-disk determinants, a direct clear comparison of the quantum mechanical cluster phase shifts of $\text{Det}\mathbf{M}(k)$ with the semiclassical ones of the Gutzwiller-Voros zeta function $Z_{GV}(k)$ is possible, which otherwise would be only small modulations on the dominating single-disk phase shifts (see [1, 33]).

In the standard cumulant expansion [see (1.8) with the Plemelj-Smithies recursion formula (1.9)] as well as in the curvature expansion [see (1.11) with (1.12)] there are large cancellations involved which become more and more dramatic the higher the cumulant order is. Let us order – without loss of generality – the eigenvalues of the trace-class operator \mathbf{A} as follows:

$$|\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_{i-1}| \geq |\lambda_i| \geq |\lambda_{i+1}| \geq \dots .$$

This is always possible because the sum over the moduli of the eigenvalues is finite for trace-class operators. Then, in the standard (Plemelj-Smithies) cumulant evaluation of the determinant there are cancellations of big numbers, e.g., at the l^{th} cumulant order ($l > 3$), all the intrinsically large “numbers” λ_1^l , $\lambda_1^{l-1}\lambda_2$, ..., $\lambda_1^{l-2}\lambda_2\lambda_3$, ... and many more have to cancel out, such that the r.h.s. of

$$\det(1 + z\mathbf{A}) = \sum_{l=0}^{\infty} z^l \sum_{j_1 < \dots < j_l} \lambda_{j_1}(\mathbf{A}) \cdots \lambda_{j_l}(\mathbf{A}). \quad (3.2)$$

is finally left over. Algebraically, the large cancellations in the exact quantum-mechanical calculation do not matter of course. However, if the determinant is calculated numerically, large cancellations might spoil the result or even the convergence. Moreover, if further approximations are made as, e.g., the transition from the exact cumulant to the semiclassical curvature expansion, these large cancellations might be potentially dangerous. Under such circumstances the underlying (algebraic) absolute convergence of the quantum-mechanical cumulant expansion cannot simply induce the

convergence of the semiclassical curvature expansion, since *large* semiclassical “errors” can completely change the convergence properties.

In summary, the non-overlapping disconnected n -disk systems have the great virtue that – although classically completely hyperbolic and for some systems even chaotic – they are quantum-mechanically *and* semiclassically “self-regulating” and also “self-unitarizing” and still simple enough that the semiclassics can be studied directly, independently of the Gutzwiller formalism, and then compared with the latter.

Acknowledgements

A.W. would like to thank the Niels-Bohr-Institute and Nordita for hospitality, and especially Predrag Cvitanović, Per Rosenqvist, Gregor Tanner, Debabrata Biswas and Niall Whelan for many discussions. M.H. would like to thank Friedrich Beck for fruitful discussions and helpful advice.

Appendix A. Existence of the n -disk \mathbf{S} -matrix and its determinant

Gaspard and Rice [4] derived in a formal way an expression for the \mathbf{S} -matrix for the 3-disk repeller. We used the same techniques in order to generalize this result to repellers consisting of n disks of *different* radii [33, 38],

$$\mathbf{S}^{(n)} = \mathbf{1} - \mathbf{i} \mathbf{T}, \quad \mathbf{T} = \mathbf{B}^j \cdot \mathbf{D}^j \quad (\text{A1})$$

$$\mathbf{C}^j = \mathbf{B}^{j'} \cdot \mathbf{M}^{j'j} \quad (\text{A2})$$

$$\mathbf{S}^{(n)} = \mathbf{1} - \mathbf{i} \mathbf{C}^j \cdot (\mathbf{M}^{-1})^{jj'} \cdot \mathbf{D}^{j'}. \quad (\text{A3})$$

$\mathbf{S}^{(n)}$ denotes the \mathbf{S} -matrix for the n -disk repeller and \mathbf{B}^j parametrizes the gradient of the wavefunction on the boundary of the disk j . The matrices \mathbf{C} and \mathbf{D} describe the coupling of the incoming and outgoing scattering waves, respectively, to the disk j and the matrix \mathbf{M} is the genuine multi-disk “scattering” matrix with eliminated single-disk properties. \mathbf{C} , \mathbf{D} and \mathbf{M} are given by eqs. (2.2), (2.3) and (2.4) respectively. The derivations of the expression for \mathbf{S} -matrix (A3) and of its determinant (see section 2) are of purely formal character as all the matrices involved are of infinite size. Here, we will show that the performed operations are all well-defined. For this purpose, the trace-class (\mathcal{J}_1) and Hilbert-Schmidt (\mathcal{J}_2) operators will play a central role.

Trace class and determinants of infinite matrices

We will briefly summarize the definitions and most important properties for trace-class and Hilbert-Schmidt matrices and operators and for determinants over infinite dimensional matrices, refs. [39, 49, 50, 51, 52] should be consulted for details and proofs.

An operator \mathbf{A} is called **trace class**, $\mathbf{A} \in \mathcal{J}_1$, if and only if, for every orthonormal basis, $\{\phi_n\}$:

$$\sum_n |\langle \phi_n, \mathbf{A} \phi_n \rangle| < \infty . \quad (\text{A4})$$

An operator \mathbf{A} is called **Hilbert-Schmidt**, $\mathbf{A} \in \mathcal{J}_2$, if and only if, for every orthonormal basis, $\{\phi_n\}$:

$$\sum_n \|\mathbf{A} \phi_n\|^2 < \infty . \quad (\text{A5})$$

The most important properties of the trace and Hilbert-Schmidt classes can be summarized as (see [39, 50]): (a) \mathcal{J}_1 and \mathcal{J}_2 are $*$ ideals., i.e., they are vector spaces closed under scalar multiplication, sums, adjoints, and multiplication with bounded operators. (b) $\mathbf{A} \in \mathcal{J}_1$ if and only if $\mathbf{A} = \mathbf{B}\mathbf{C}$ with $\mathbf{B}, \mathbf{C} \in \mathcal{J}_2$. (c) For any operator \mathbf{A} , we have $\mathbf{A} \in \mathcal{J}_2$ if $\sum_n \|\mathbf{A} \phi_n\|^2 < \infty$ for a single basis. (d) For any operator $\mathbf{A} \geq 0$, we have $\mathbf{A} \in \mathcal{J}_1$ if $\sum_n |\langle \phi_n, \mathbf{A} \phi_n \rangle| < \infty$ for a single basis.

Let $\mathbf{A} \in \mathcal{J}_1$, then the determinant $\det(\mathbf{1} + z\mathbf{A})$ exists [39, 49, 50, 51, 52], it is an entire and analytic function of z and it can be expressed by the *Plemelj-Smithies formula*: Define $\alpha_m(\mathbf{A})$ for $\mathbf{A} \in \mathcal{J}_1$ by

$$\det(\mathbf{1} + z\mathbf{A}) = \sum_{m=0}^{\infty} z^m \frac{\alpha_m(\mathbf{A})}{m!} . \quad (\text{A6})$$

Then $\alpha_m(\mathbf{A})$ is given by the $m \times m$ determinant

$$\alpha_m(\mathbf{A}) = \begin{vmatrix} \text{Tr}(\mathbf{A}) & m-1 & 0 & \cdots & 0 \\ \text{Tr}(\mathbf{A}^2) & \text{Tr}(\mathbf{A}) & m-2 & \cdots & 0 \\ \text{Tr}(\mathbf{A}^3) & \text{Tr}(\mathbf{A}^2) & \text{Tr}(\mathbf{A}) & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \text{Tr}(\mathbf{A}^m) & \text{Tr}(\mathbf{A}^{(m-1)}) & \text{Tr}(\mathbf{A}^{(m-2)}) & \cdots & \text{Tr}(\mathbf{A}) \end{vmatrix} \quad (\text{A7})$$

with the understanding that $\alpha_0(\mathbf{A}) \equiv 1$ and $\alpha_1(\mathbf{A}) \equiv \text{Tr}(\mathbf{A})$. Thus the cumulants $c_m(\mathbf{A}) \equiv \alpha_m(\mathbf{A})/m!$ (with $c_0(\mathbf{A}) \equiv 1$) satisfy the recursion relation

$$c_m(\mathbf{A}) = \frac{1}{m} \sum_{k=1}^m (-1)^{k+1} c_{m-k}(\mathbf{A}) \text{Tr}(\mathbf{A}^k) \quad \text{for } m \geq 1 .$$

The most important properties of these determinants are: (i) If $\mathbf{A}, \mathbf{B} \in \mathcal{J}_1$, then $\det(\mathbf{1} + \mathbf{A}) \det(\mathbf{1} + \mathbf{B}) = \det(\mathbf{1} + \mathbf{A} + \mathbf{B} + \mathbf{A}\mathbf{B}) = \det[(\mathbf{1} + \mathbf{A})(\mathbf{1} + \mathbf{B})] = \det[(\mathbf{1} + \mathbf{B})(\mathbf{1} + \mathbf{A})]$. (ii) If $\mathbf{A} \in \mathcal{J}_1$ and \mathbf{U} unitary, then $\det(\mathbf{U}^\dagger(\mathbf{1} + \mathbf{A})\mathbf{U}) = \det(\mathbf{1} + \mathbf{U}^\dagger \mathbf{A} \mathbf{U}) = \det(\mathbf{1} + \mathbf{A})$. (iii) If $\mathbf{A} \in \mathcal{J}_1$, then $(\mathbf{1} + \mathbf{A})$ is invertible if and only if $\det(\mathbf{1} + \mathbf{A}) \neq 0$. (d) For any $\mathbf{A} \in \mathcal{J}_1$,

$$\det(\mathbf{1} + \mathbf{A}) = \prod_{j=1}^{N(\mathbf{A})} [1 + \lambda_j(\mathbf{A})] , \quad (\text{A8})$$

where here and in the following $\{\lambda_j(\mathbf{A})\}_{j=1}^{N(\mathbf{A})}$ are the eigenvalues of \mathbf{A} counted with algebraic multiplicity ($N(\mathbf{A})$ can of course be infinite).

Now we can return to the actual problem. The $\mathbf{S}^{(n)}$ -matrix is given by (A1). The \mathbf{T} -matrix is trace-class on the positive real k axis ($k > 0$), as it is the product of the matrices \mathbf{D}^j and \mathbf{B}^j which will turn out to be trace-class or, respectively, bounded there (see [39, 49] for the definitions). Again formally, we have used that $\mathbf{C}^j = \mathbf{B}^{j'} \mathbf{M}^{j'j}$ implies the relation $\mathbf{B}^{j'} = \mathbf{C}^j (\mathbf{M}^{-1})^{jj'}$. Thus, the existence of $\mathbf{M}^{-1}(k)$ has to be shown, too – except at isolated poles in the lower complex k plane below the real k axis and on the branch cut on the negative real k axis which results from the branch cut of the defining Hankel functions. As we will prove later, $\mathbf{M}(k) - \mathbf{1}$ is trace-class, except of course at the above mentioned points in the k plane. Therefore, using property (iii), we only have to show that $\text{Det} \mathbf{M}(k) \neq 0$ in order to guarantee the existence of $\mathbf{M}^{-1}(k)$. At the same time, $\mathbf{M}^{-1}(k)$ will be proven to be bounded as all its eigenvalues and the product of its eigenvalues are then finite. The existence of these eigenvalues follows from the trace-class property of $\mathbf{M}(k)$ which together with $\text{Det} \mathbf{M}(k) \neq 0$ guarantees the finiteness of the eigenvalues and their product [39, 49].

We have normalized \mathbf{M} in such a way that we simply have $\mathbf{B} = \mathbf{C}$ for the scattering from a single disk. Note that the structure of the matrix \mathbf{C}^j does not depend on the fact whether the point particle scatters only from a single disk or from n disks. The functional form (2.2) shows that \mathbf{C} cannot have poles on the real positive k axis ($k > 0$) in agreement with the structure of the $\mathbf{S}^{(1)}$ -matrix [see equation (2.7)]. If the origin of the coordinate system is put into the origin of the disk, the matrix $\mathbf{S}^{(1)}$ is diagonal. In the same basis \mathbf{C} becomes diagonal. One can easily see that \mathbf{C} has no zero eigenvalue on the positive real k axis and that it will be trace-class. So neither \mathbf{C} nor the 1-disk (or for that purpose the n -disk) \mathbf{S} matrix can possess poles or zeros on the real positive k axis. The statement about $\mathbf{S}^{(n)}$ follows simply from the unitarity of the \mathbf{S} -matrix which can be checked easily. The fact that $|\det \mathbf{S}^{(n)}(k)| = 1$ on the positive real k axis cannot be used to disprove that $\text{Det} \mathbf{M}(k)$ could be zero there [see equation (2.8)]. However, if $\text{Det} \mathbf{M}(k)$ were zero there, this “would-be” pole must cancel out of $\mathbf{S}^{(n)}(k)$. Looking at formula (A3), this pole has to cancel out against a zero from \mathbf{C} or \mathbf{D} where both matrices are already fixed on the 1-disk level. Now, it follows from (A8) that $\mathbf{M}(k)$ (provided that $\mathbf{M} - \mathbf{1}$ has been proven trace-class) has only one chance to make trouble on the positive real k axis, namely, if at least one of its eigenvalues (whose existence is guaranteed) becomes zero. On the other hand \mathbf{M} has still to satisfy $\mathbf{C}^j = \mathbf{B}^{j'} \mathbf{M}^{j'j}$. Comparing the left and the right-hand side of $|\mathbf{C}_{mm}^j(k)| = |\mathbf{B}_{ml}^{j'} \mathbf{M}_{lm}^{j'j}|$ in the eigenbasis of \mathbf{M} and having in mind that $\mathbf{C}^j(k)$ cannot have zero eigenvalue for $k > 0$ one finds a contradiction if the corresponding eigenvalue of $\mathbf{M}(k)$ were zero. Hence $\mathbf{M}(k)$ is invertible on the real positive k axis, provided, as mentioned now several times,

$\mathbf{M}(k) - \mathbf{1}$ is trace-class. From the existence of the inverse relation $\mathbf{B}^{j'} = \mathbf{C}^j(\mathbf{M}^{-1})^{jj'}$ and the to be shown trace-class property of \mathbf{C}^j and the boundedness of $(\mathbf{M}^{-1})^{jj'}$ follows the boundedness of \mathbf{B}^j and therefore the trace-class property of the n -disk \mathbf{T} -matrix, $\mathbf{T}^{(n)}(k)$, except at the above excluded k -values.

What is left for us to do is to prove

- (a) $\mathbf{M}(k) - \mathbf{1} \in \mathcal{J}_1$ for all k , except at the poles of $H_m^{(1)}(ka_j)$ and for $k \leq 0$,
- (b) $\mathbf{C}^j(k), \mathbf{D}^j(k) \in \mathcal{J}_1$ with the exception of the same k -values mentioned in (a),
- (c) $\mathbf{T}^{(1)}(ka_j) \in \mathcal{J}_1$ (again with the same exceptions as in (a)) where $\mathbf{T}^{(1)}$ is the \mathbf{T} -matrix of the 1-disk problem,
- (d) $\mathbf{M}^{-1}(k)$ does not only exist, but is bounded.

Under these conditions all the manipulations of section 2 [equations (2.5) and (2.8)] are justified and $\mathbf{S}^{(n)}$, as in (2.1), and $\det \mathbf{S}^{(n)}$, as in (2.8), are shown to exist.

Proof of $\mathbf{T}^{(1)}(ka_j) \in \mathcal{J}_1$

The \mathbf{S} -Matrix for the j^{th} disk is given by

$$\mathbf{S}_{ml}^{(1)}(ka_j) = -\frac{H_l^{(2)}(ka_j)}{H_l^{(1)}(ka_j)}\delta_{ml}. \quad (\text{A9})$$

Thus $\mathbf{V} \equiv -i \mathbf{T}^{(1)}(ka_j) = \mathbf{S}^{(1)}(ka_j) - \mathbf{1}$ is diagonal. Hence, we can write $\mathbf{V} = \mathbf{U}|\mathbf{V}|$ where \mathbf{U} is diagonal and unitary, and therefore bounded. What is left to show is that $|\mathbf{V}| \in \mathcal{J}_1$. We just have to show in a special orthonormal basis (the eigenbasis) that

$$\sum_{l=-\infty}^{+\infty} |\mathbf{V}|_{ll} = \sum_{l=-\infty}^{+\infty} 2 \left| \frac{J_l(ka_j)}{H_l^{(1)}(ka_j)} \right| < \infty, \quad (\text{A10})$$

since $|\mathbf{V}| \geq 0$ by definition (see property (d)). The convergence of this series can be shown easily using the asymptotic formulae for Bessel and Hankel functions for large orders, $\nu \rightarrow \infty$, ν real:

$$J_\nu(ka) \sim \frac{1}{\sqrt{2\pi\nu}} \left(\frac{eka}{2\nu} \right)^\nu, \quad H_\nu^{(1)}(ka) \sim -i \sqrt{\frac{2}{\pi\nu}} \left(\frac{eka}{2\nu} \right)^{-\nu} \quad (\text{A11})$$

(see e.g. [53]). From this equation follows the mathematical justification for the impact parameter (or angular momentum) truncation in the semiclassical resolution of the *single* disks, $|m| \leq \frac{\epsilon}{2}ka$. This limit should not be confused with the truncation in the curvature order resulting from the finite resolution of the repelling set of the n -disk problem, see ref. [1]. Under these asymptotic formulae and the summation of the resulting geometrical series, the trace-class property of $|\mathbf{V}| \in \mathcal{J}_1$ and $\mathbf{S}^{(1)} - \mathbf{1} \in \mathcal{J}_1$ follows immediately. That in turn means that $\det \mathbf{S}^{(1)}(ka_j)$ exists and also that the product $\prod_{j=1}^n \det \mathbf{S}^{(1)}(ka_j) < \infty$ if n is finite (see [39, 49]). Note that the limit $n \rightarrow \infty$ does not exist in general.

Proof of $\mathbf{A}(k) \equiv \mathbf{M}(k) - \mathbf{1} \in \mathcal{J}_1$

The determinant of the characteristic matrix $\mathbf{M}(k)$ is defined, if $\mathbf{A}(k) \in \mathcal{J}_1$. In order to show this, we split \mathbf{A} into the product of two operators which – as we will show – are both Hilbert-Schmidt. Then the product is trace-class (see property (b)).

Let therefore $\mathbf{A} = \mathbf{E} \cdot \mathbf{F}$ with $\mathbf{A} = \mathbf{M} - \mathbf{1}$ as given in (2.4). In order to simplify the decomposition of \mathbf{A} , we choose one of the factors, namely, \mathbf{F} , as a diagonal matrix. Let therefore

$$\mathbf{F}_{ll'}^{jj'} = \frac{\sqrt{H_{2l}^{(1)}(k\alpha a_j)}}{H_l^{(1)}(ka_j)} \delta^{jj'} \delta_{ll'} , \quad \alpha > 2 . \quad (\text{A12})$$

This ansatz already excludes the zeros of the Hankel functions $H_l^{(1)}(ka_j)$ and also the negative real k axis (the branch cut of the Hankel functions for $k \leq 0$) from our final proof of $\mathbf{A}(k) \in \mathcal{J}_1$. First, we have to show that $\|\mathbf{F}\|^2 = \sum_j \sum_l (\mathbf{F}^\dagger \mathbf{F})_{ll}^{jj} < \infty$. We start with

$$\|\mathbf{F}\|^2 \leq \sum_{j=1}^n 2 \sum_{l=0}^{\infty} \frac{|H_{2l}^{(1)}(k\alpha a_j)|}{|H_l^{(1)}(ka_j)|^2} \equiv \sum_{j=1}^n 2 \sum_{l=0}^{\infty} a_l . \quad (\text{A13})$$

This expression restricts our proof to n -disk configurations with n finite. Using the asymptotic expressions for the Bessel and Hankel functions of large orders (A11) (see e.g. [53]), it is easy to prove the absolute convergence of $\sum_l a_l$ in the case $\alpha > 2$. Therefore $\|\mathbf{F}\|^2 < \infty$ and because of property (c) we get $\mathbf{F} \in \mathcal{J}_2$.

We now investigate the second factor \mathbf{E} . We have to show the convergence of

$$\|\mathbf{E}\|^2 = \sum_{\substack{j,j'=1 \\ j \neq j'}}^n \left(\frac{a_j}{a_{j'}} \right)^2 \sum_{l,l'=-\infty}^{\infty} a_{ll'} , \quad a_{ll'} = \frac{|J_l(ka_j)|^2 |H_{l-l'}^{(1)}(kR_{jj'})|^2}{|H_{2l}^{(1)}(k\alpha a_{j'})|} \quad (\text{A14})$$

in order to prove that also $\mathbf{E} \in \mathcal{J}_2$. Using the same techniques as before the convergence of $\sum_l a_{ll'}$ for $(1+\epsilon)a_j < R_{jj'}$, $\epsilon > 0$, as well as the convergence of $\sum_{l'} a_{ll'}$ for $\alpha a_{j'} < 2R_{jj'}$, $\alpha > 2$, can be shown. We must of course show the convergence of $\sum_{l,l'} a_{ll'}$ for the case $l, l' \rightarrow \infty$ as well. Under the asymptotic behavior of the Bessel and Hankel functions of large order (A11), it is easy to see that it suffices to prove the convergence of $\sum_{l,l'=0}^{\infty} b_{ll'}$, where

$$b_{ll'} = \frac{(l+l')^{2(l+l')}}{l^{2l} l'^{2l'}} \left(\frac{a_j}{R_{jj'}} \right)^{2l} \left(\frac{\alpha a_{j'}}{2 R_{jj'}} \right)^{2l'} . \quad (\text{A15})$$

In order to show the convergence of the double sum, we introduce new summation indices (M, m) , namely $2M := l + l'$ and $m := l - l'$. Using first Stirling's formula for large powers M and then applying the binomial formula in order to perform the summation over m , the convergence of $\sum_{l,l'=0}^{\infty} b_{ll'}$ can be shown, provided that $a_j + \frac{\alpha}{2} a_{j'} < R_{jj'}$. Under

this condition the operator \mathbf{E} belongs to the class of Hilbert–Schmidt operators (\mathcal{J}_2). In summary, this means: $\mathbf{E}(\mathbf{k}) \cdot \mathbf{F}(\mathbf{k}) = \mathbf{A}(k) \in \mathcal{J}_1$ for those n disk configurations for which the number of disks is finite and the disks neither overlap nor touch and for those values of k which lie neither on the zeros of the Hankel functions $H_m^{(1)}(ka_j)$ nor on the negative real k axis ($k \leq 0$). The zeros of the Hankel functions $H_m^{(2)}(k^*a_j)$ are then automatically excluded, too. The zeros of the Hankel functions $H_m^{(1)}(k\alpha a_j)$ in the definition of \mathbf{E} are cancelled by the corresponding zeros of the same Hankel functions in the definition of \mathbf{F} and can therefore be removed, i.e., a slight change in α readjusts the positions of the zeros in the complex k plane such that they can always be moved to non-dangerous places.

Proof of $\mathbf{C}^j, \mathbf{D}^j \in \mathcal{J}_1$

The expressions for \mathbf{D}^j and \mathbf{C}^j can be found in (2.3) and (2.2). Both matrices contain – for a fixed value of j – only the information of the single disk scattering. As in the proof of $\mathbf{T}^{(1)} \in \mathcal{J}_1$, we go to the eigenbasis of $\mathbf{S}^{(1)}$. In that basis both matrices \mathbf{D}^j and \mathbf{C}^j become diagonal. Using the same techniques as in the proof of $\mathbf{T}^{(1)} \in \mathcal{J}_1$, we can show that \mathbf{C}^j and \mathbf{D}^j are trace-class. In summary, we have $\mathbf{D}^j \in \mathcal{J}_1$ for all k as the Bessel functions which define that matrix possess neither poles nor branch cuts. The matrix \mathbf{C}^j is traceclass for almost every k , except at the zeros of the Hankel functions $H_m^{(1)}(ka_j)$ and the branch cut of these Hankel functions on the negative real k axis ($k \leq 0$).

Existence and boundedness of $\mathbf{M}^{-1}(k)$

$\text{Det}\mathbf{M}(k)$ exists almost everywhere, since $\mathbf{M}(k) - \mathbf{1} \in \mathcal{J}_1$, except at the zeros of $H_m^{(1)}(ka_j)$ and on the negative real k axis ($k \leq 0$). Modulo these points $\mathbf{M}(k)$ is analytic. Hence, the points of the complex k plane with $\text{Det}\mathbf{M}(k) = 0$ are isolated. Thus almost everywhere $\mathbf{M}(k)$ can be diagonalized and the product of the eigenvalues weighted by their degeneracies is finite and nonzero. Hence, where $\text{Det}\mathbf{M}(k)$ is defined and nonzero, $\mathbf{M}^{-1}(k)$ exists, it can be diagonalized and the product of its eigenvalues is finite. In summary, $\mathbf{M}^{-1}(k)$ is bounded and $\text{Det}\mathbf{M}^{-1}(k)$ exists almost everywhere in the complex k plane.

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